BUSSTEPP Homework 3: More Exercises on Numerical Quantum Mechanics Other Exercises

September 2, 2003

1 Numerical Exercises

1.1 Harmonic Oscillator

We continue with the harmonic oscillator,

$$V(x) = \tfrac{1}{2}m\omega^2 x^2, \tag{1}$$

$$S = ma\left\{\sum_{i=0}^{N-1} \tfrac{1}{2}[x_{i+1} - x_i)/a]^2 + \tfrac{1}{2}(\omega a)^2(x_i/a)^2\right\}. \tag{2}$$

Exercise III.1: Run with the parameters in Table 1 to vary the lattice spacing. Plot E_1, E_2, and E_2/E_1 vs. a. Verify also that the energies do not depend on m. Results are in Fig. 1.

Explain the striking constancy of $E_2/E_1 = 2$.

Solution III.1: The canned programs require somewhat different input (a, τ, N):

a	0.5	1	2	4	8
τ/π	2	2	2	2	2
N	128	64	32	16	8

Make a directory for each parameter set, with appropriate input files, abtain E_1 and E_2 from effective masses.

Because the system is quadratic, we can solve for all eigenvalues of the transfer operator. First set $x = q\sqrt{a/m}$, which scales m out of the problem. The transfer operator:

$$(\hat{\mathbb{T}}\Psi)_n(q_{t+1}) = \int \frac{dq_t}{\sqrt{2\pi}}\ \exp\left\{-\tfrac{1}{2}[1+\tfrac{1}{2}(\omega a)^2]q_{t+1}^2 + q_{t+1}q_t - \tfrac{1}{2}[1+\tfrac{1}{2}(\omega a)^2]q_t^2\right\}\Psi(x_t)$$

The simple harmonic oscillator has wave functions

$$\Psi_n(q) = \mathcal{N}_n e^{\alpha^2 q^2}\int \frac{du}{\sqrt{2\pi}}\ u^n e^{-\frac{1}{2}u^2 + 2i\alpha u q},$$

Table 1: Parameters for exploring the dependence on a.

ma	0.5	1	1.5	2	3
ωa	0.5	1	1.5	2	3
N	128	64	44	32	22

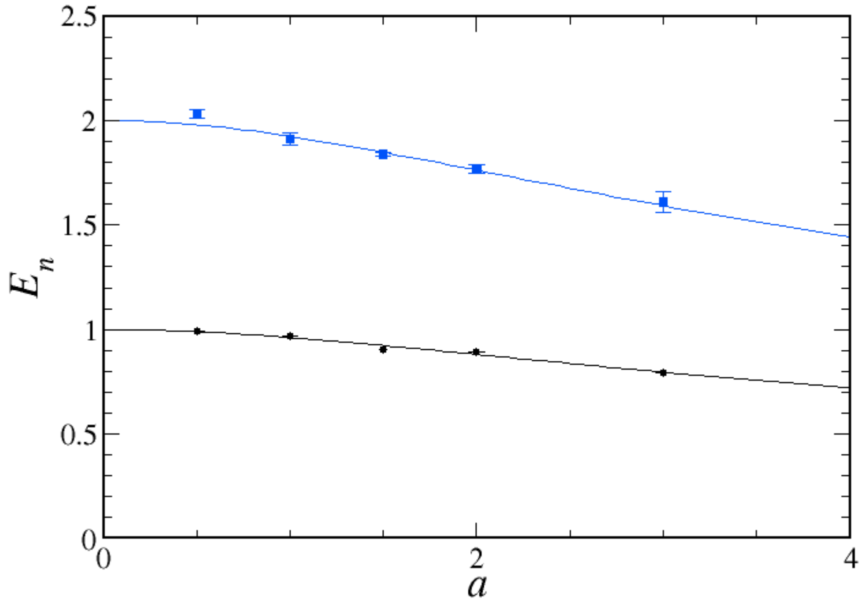

Figure 1: E_1 and E_2 vs. lattice spacing a. The points are Monte Carlo simulation. The lines are the exact solution at non-zero a.

choosing an integral representation, because we have $\mathbb{T}$ in an integral representation. For now α is not known. A straightforward, but tedious, manipulation of Gaussian integrals shows that Ψ_n is an eigenfunction of $\hat{\mathbb{T}}$ with eigenvalue

$$\mathbb{T}_n = e^{-(n+\frac{1}{2})Ea},$$

where

$$\cosh(Ea) = 1 + \tfrac{1}{2}(\omega a)^2 \qquad \Rightarrow \qquad Ea = 2\sinh^{-1}(\tfrac{1}{2}\omega a).$$

One finds that this works out if $\alpha^2 = 2\sinh(Ea)$.

Thus, all the discretization effect can be absorbed into a redefinition of the frequency.

1.2 Anharmonic Oscillator

Now add an anharmonic term

$$V(x) = \tfrac{1}{2}m\omega^2x^2 + \lambda x^4, \tag{3}$$

$$S = ma\left\{\sum_{i=0}^{N-1} \tfrac{1}{2}[x_{i+1} - x_i)/a]^2 + \tfrac{1}{2}(\omega a)^2(x_i/a)^2 + (\lambda a^5/ma)(x_i/a)^4\right\}. \tag{4}$$

From first-order perturbation theory

$$E_n = n\omega\left(1 + \frac{3\lambda(n+1)}{2m^2\omega^3}\right) \tag{5}$$

so the correction is small if $\lambda \ll m^2\omega^3$. The energies as a function of λ are shown in Fig. 2

Exercise III.2: Compute the energies E_1 and E_2 as a function of λ at a lattice spacing so that discretization effects are small. Start with λ small enough so that perturbation theory should be accurate, but extend into the non-perturbative regime.

Solution III.2: My result used $ma = \omega a = 1$ and λa^5.

1.3 Double-well Oscillator

The exercise in this subsection uses the potential

$$V(x) = -\tfrac{1}{2}m\omega^2x^2 + \lambda x^4 \tag{6}$$

Note the minus sign in front of the quadratic term. There are two minima. Now the first excited state is almost degenerate with the ground state.

Exercise III.3: Return to the program that compute $x_{\rm avg}$ as a function of c. Plot them vs. c. Explain the behavior of $x_{\rm avg}$, Fig. **??**.

Solution III.3: So far I have not found a set of simulation parameters such that the system switches back and forth. If you find some, e-mail `ask@fnal.gov`

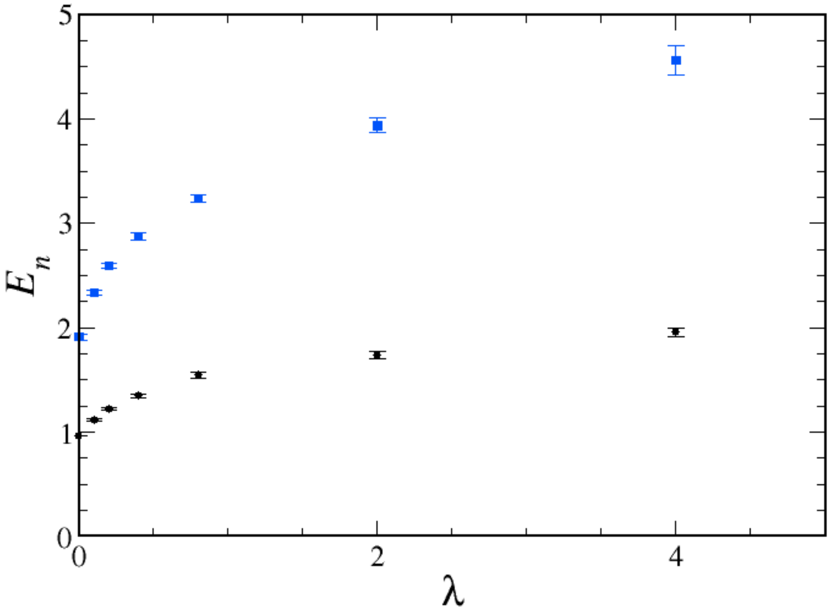

Figure 2: E_1 and E_2 vs. anharmonicity λ, in lattice units.

2 Other Exercises

The Standard Yukawa interactions of quarks are

$$\mathcal{L}_Y = -\sum_{i,j=1}^{G}\left[\hat{y}^d_{ij}\bar{Q}^i_L\phi\, D^j_R + \hat{y}^u_{ij}\bar{Q}^i_L\tilde{\phi}\, U^j_R + \text{h.c.}\right], \tag{7}$$

with hypercharges $Y_U = 2/3$, $Y_D = -1/3$, $Y_Q = 1/6$.

Exercise III.4: What must the hypercharge of the Higgs doublet(s) be?

Solution III.4:

$$\begin{aligned} Y_\phi &= 1/3 + 1/6 = 1/2 \\ Y_{\tilde{\phi}} &= -2/3 + 1/6 = -1/2 \end{aligned}$$

In continuum gauge theories the parallel transporter (or Wilson line) is defined to be

$$U(x,y) = \mathsf{P}\exp\left(\int_y^x dz\cdot A\right). \tag{8}$$

Exercise III.5: Show that $U(x,y) \to g(x)U(x,y)g^{-1}(y)$ under gauge transformations.

Solution III.5: The proof is immediate for an infinitesimally short path. Any path can be built out of short paths, by definition of the path-ordering symbol.

The Wilson plaquette action is

$$S = \frac{\beta}{2N}\sum_{x,\mu,\nu} P_{\mu\nu}(x) \tag{9}$$

where

$$P_{\mu\nu} = \mathrm{Re}\,\mathrm{tr}[1 - U_\mu(x)U_\nu(x+ae^{(\mu)})U^\dagger_\mu(x+ae^{(\nu)})U^\dagger_\nu(x)]. \tag{10}$$

Exercise III.6: Show that the plaquette action reduces to the Yang-Mills action when $a \to 0$.

Solution III.6: It is convenient to focus on a single $\mu\nu$ plaquette, located (for convenience) at the origin 0. Choose a gauge so that $A_\nu(x) = 0$. Fix the gauge further so that on the hypersurface $x_\nu = 0$ $A_\mu(x) = 0$ too. Then

$$P_{\mu\nu}(0) = \mathrm{Re}\,\mathrm{tr}[1 - U^\dagger_\mu(ae^{(\nu)})] = \mathrm{Re}\,\mathrm{tr}\{1 - P\exp[-a\int_0^1 A_\mu(sae^{(\nu)})ds]\}$$

Now in this gauge

$$A_\mu(sae^{(\nu)}) = A_\mu(0) + sa\partial_\nu A_\mu = sa\partial_\nu A_\mu$$

because $A_\mu(0) = 0$ when $x_\nu = 0$. The first term to survive the trace is the second order in $sa\partial_\nu A_\mu$:

$$P_{\mu\nu}(0) = -a^4 \mathrm{Re}\,\mathrm{tr}[\tfrac{1}{2}(\partial_\nu A_\mu(0))^2] == -a^4\tfrac{1}{2}\,\mathrm{tr}[(F_{\nu\mu}(0))^2]$$

The last equality holds in our gauge $F_{\nu\mu}(0) = \partial_\nu A_\mu$. Since the left-most and right-most expressions are both gauge invariant, they hold in all gauges.

Next repeat for all plaquettes, yielding

$$P_{\mu\nu}(x) = -a^4\tfrac{1}{2}\,\mathrm{tr}[(F_{\nu\mu}(x))^2] = +\frac{1}{4}\sum_a (F^a_{\mu\nu})^2$$

no sum on $\mu\nu$. With my convention for the generators $\mathrm{tr}[t^a t^b] = -\tfrac{1}{2}\delta^{ab}$.

Thus

$$\sum_{x,\mu,\nu} P_{\mu\nu}(x) = a^4 \sum_x \frac{1}{4}(F^a_{\mu\nu}(x))^2 = \int d^4x \frac{1}{4}(F^a_{\mu\nu}(x))^2$$

with summation conventions on the right-hand side. Normalization indentifies $\beta/2N = 1/g_0^2$.